

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.89	0.25	0.88	0.26	0.75	0.38

Model Results

Predicted value: 4.68 days

Global applicability domain: Inside

Local applicability domain index: 6.41e-01

Confidence level: 8.01e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>1,3,5-Trimethylbenzene</div> <div>Measured: 12.5</div> <div>Predicted: 3.63</div>	<div>Image not found</div> <div>1,2,4,5-Tetramethylbenzene</div> <div>Measured: 88.3</div> <div>Predicted: 5.46</div>	<div>Image not found</div> <div>para-Xylene</div> <div>Measured: 157</div> <div>Predicted: 5.33</div>
<div>Image not found</div> <div>1,2,3,5-Tetramethylbenzene</div> <div>Measured: 12.5</div> <div>Predicted: 3.31</div>	<div>Image not found</div> <div>Methylcyclohexane</div> <div>Measured: 24.3</div> <div>Predicted: 4.12</div>	